```
* * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:55:50 ON 30 JAN 2006

=> file reg
COST IN U.S. DOLLARS                              SINCE FILE       TOTAL
                                                    ENTRY         SESSION
FULL ESTIMATED COST                                  0.21          0.21

FILE 'REGISTRY' ENTERED AT 09:56:01 ON 30 JAN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   27 JAN 2006  HIGHEST RN 872965-93-0
DICTIONARY FILE UPDATES:  27 JAN 2006  HIGHEST RN 872965-93-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\0508791.str

L1        STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1                    STR
```
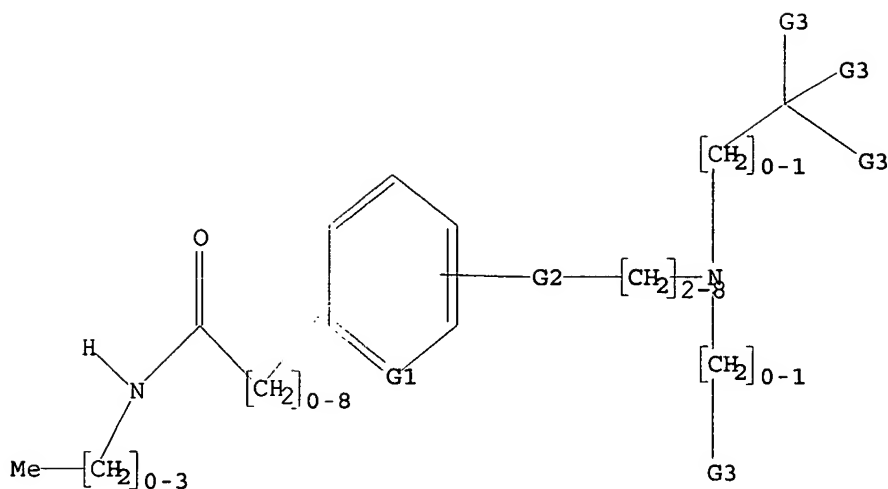
G1 C,N

G2 C,O,S,N

G3 Cb,Cy,Hy,H

Structure attributes must be viewed using STN Express query preparation.


```
=> s l1
SAMPLE SEARCH INITIATED 09:56:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   208278 TO ITERATE

   1.0% PROCESSED      2000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:   ONLINE   **INCOMPLETE**
                         BATCH    **INCOMPLETE**
PROJECTED ITERATIONS:       4138858 TO   4192262
PROJECTED ANSWERS:                0 TO          0

L2              0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 09:56:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   4157575 TO ITERATE

  10.7% PROCESSED    445300 ITERATIONS   (      1 INCOMPLETE)      18 ANSWERS

  19.2% PROCESSED    799368 ITERATIONS   (      1 INCOMPLETE)      38 ANSWERS

  22.5% PROCESSED    933850 ITERATIONS   (      1 INCOMPLETE)      45 ANSWERS

  24.1% PROCESSED   1000000 ITERATIONS   (      1 INCOMPLETE)      48 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.57

FULL FILE PROJECTIONS:   ONLINE   **INCOMPLETE**
                         BATCH    **INCOMPLETE**
PROJECTED ITERATIONS:       4157575 TO   4157575
PROJECTED ANSWERS:              157 TO        241

L3              48 SEA SSS FUL L1

=> d l3 1-48

L3    ANSWER 1 OF 48  REGISTRY  COPYRIGHT 2006 ACS on STN
RN    864911-65-9  REGISTRY
ED    Entered STN:  11 Oct 2005
CN    Propanamide, 3-[[[4-[[bis(1H-imidazol-2-ylmethyl)amino]methyl]phenyl]methy
```
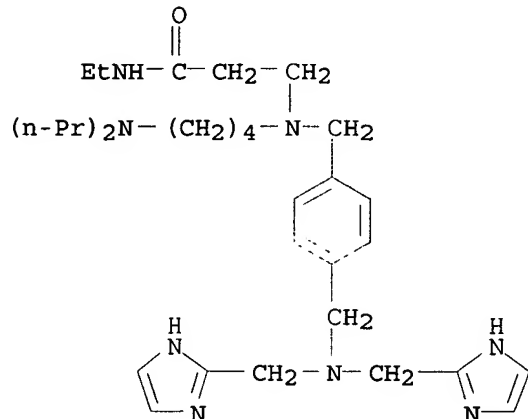
1] [4-(dipropylamino)butyl]amino]-N-ethyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C31 H50 N8 O
SR   CA
LC   STN Files: CA, CAPLUS

$$EtNH-\overset{\overset{\textstyle O}{\|}}{C}-CH_2-CH_2$$

(n-Pr)$_2$N—(CH$_2$)$_4$—N—CH$_2$

CH$_2$—N—CH$_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

            1 REFERENCES IN FILE CA (1907 TO DATE)
            1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 2 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN   864911-57-9 REGISTRY
ED   Entered STN: 11 Oct 2005
CN   Propanamide, 3-[[4-(dipropylamino)butyl][[4-[[[(1H-imidazol-2-ylmethyl)[(1-
      methyl-1H-imidazol-2-yl)methyl]amino]methyl]phenyl]methyl]amino]-N-ethyl-
      (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C32 H52 N8 O
SR   CA
LC   STN Files: CA, CAPLUS
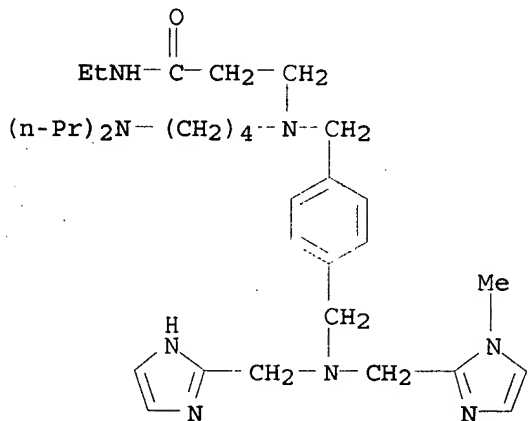
$$EtNH-\overset{\overset{\textstyle O}{\|}}{C}-CH_2-CH_2$$

(n-Pr)$_2$N—(CH$_2$)$_4$—N—CH$_2$

CH$_2$

CH$_2$—N—CH$_2$

Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

            1 REFERENCES IN FILE CA (1907 TO DATE)
            1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 3 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN   864782-53-6 REGISTRY
ED   Entered STN: 07 Oct 2005
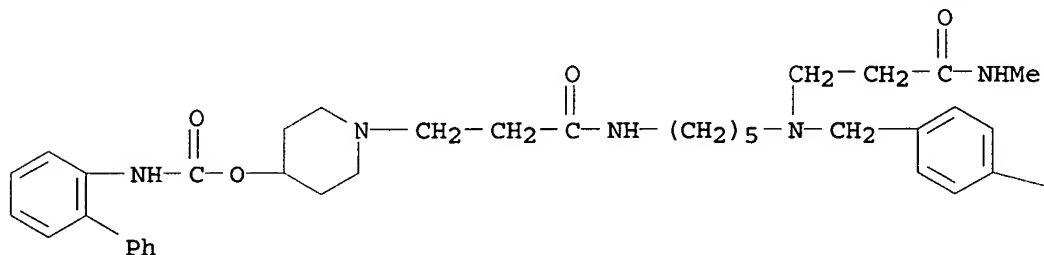CN   Carbamic acid, [1,1'-biphenyl]-2-yl-, 1-[3-[[5-[[(4-

hydroxyphenyl)methyl] [3-(methylamino)-3-oxopropyl]amino]pentyl]amino]-3-
oxopropyl]-4-piperidinyl ester, trifluoroacetate (salt) (9CI)   (CA INDEX
NAME)
MF   C37 H49 N5 O5 . x C2 H F3 O2
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL

CM   1

CRN   864782-52-5
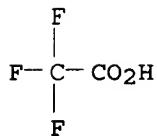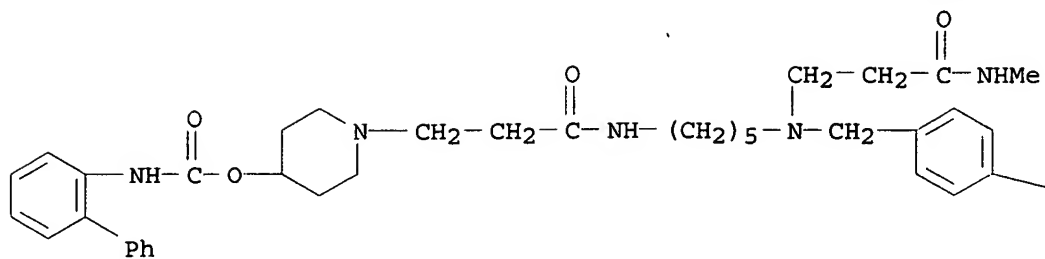CMF   C37 H49 N5 O5

PAGE 1-A

PAGE 1-B

—OH

CM   2

CRN   76-05-1
CMF   C2 H F3 O2

        1 REFERENCES IN FILE CA (1907 TO DATE)
        1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 4 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   864782-52-5   REGISTRY
ED   Entered STN: 07 Oct 2005
CN   Carbamic acid, [1,1'-biphenyl]-2-yl-, 1-[3-[[5-[[(4-
      hydroxyphenyl)methyl] [3-(methylamino)-3-oxopropyl]amino]pentyl]amino]-3-
      oxopropyl]-4-piperidinyl ester (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C37 H49 N5 O5
CI   COM
SR   CA
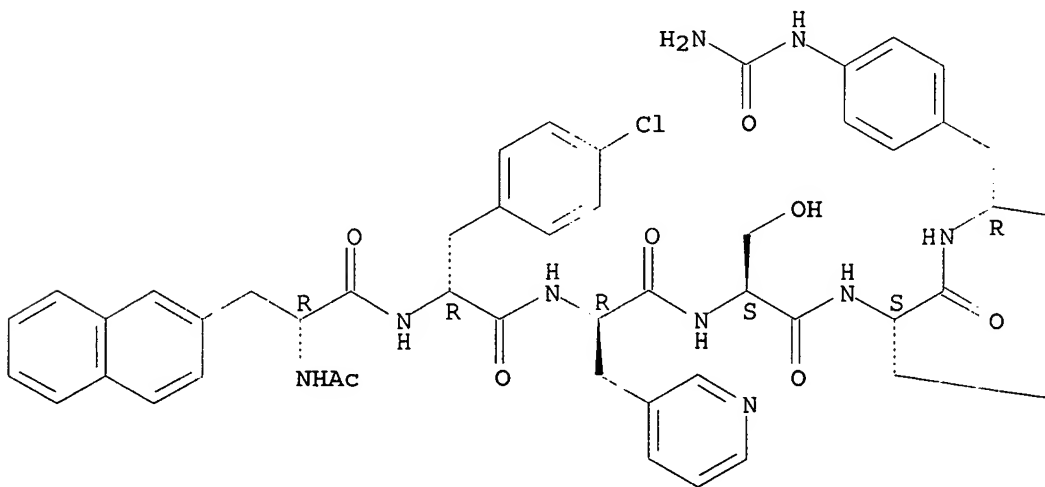LC   STN Files: CA, CAPLUS, USPATFULL

—OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT
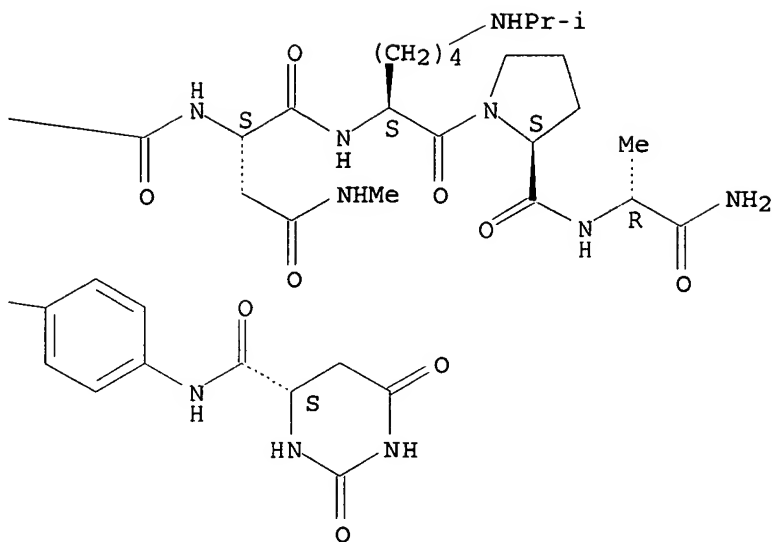
          1 REFERENCES IN FILE CA (1907 TO DATE)
          1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 5 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   862993-48-4   REGISTRY
ED   Entered STN: 13 Sep 2005
CN   D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-D-
      phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-4-[[[(4S)-hexahydro-2,6-
      dioxo-4-pyrimidinyl]carbonyl]amino]-L-phenylalanyl-4-
      [(aminocarbonyl)amino]-D-phenylalanyl-N-methyl-L-asparaginyl-N6-(1-
      methylethyl)-L-lysyl-L-prolyl- (9CI)   (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
MF   C81 H100 Cl N19 O17
SR   CA
LC   STN Files: CA, CAPLUS, CASREACT

RELATED SEQUENCES AVAILABLE WITH SEQLINK
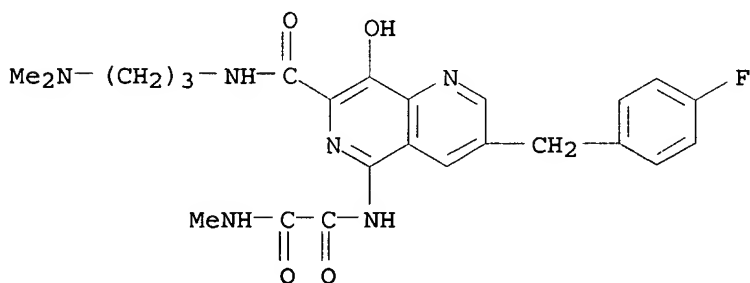
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

     1 REFERENCES IN FILE CA (1907 TO DATE)
     1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 6 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN   862508-84-7 REGISTRY
ED   Entered STN: 06 Sep 2005
CN   Ethanediamide, N-[7-[[[3-(dimethylamino)propyl]amino]carbonyl]-3-[(4-
     fluorophenyl)methyl]-8-hydroxy-1,6-naphthyridin-5-yl]-N'-methyl- (9CI)
     (CA INDEX NAME)
FS   3D CONCORD
MF   C24 H27 F N6 O4
SR   CA
LC   STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

     1 REFERENCES IN FILE CA (1907 TO DATE)
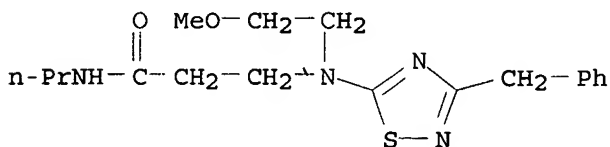   1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 7 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN   859353-37-0 REGISTRY
ED   Entered STN: 10 Aug 2005
CN   Propanamide, N-butyl-3-[butyl[3-[(4-methylphenyl)methyl]-1,2,4-thiadiazol-

FS   3D CONCORD
MF   C21 H32 N4 O S
SR   Chemical Library
         Supplier: ComGenex International Inc.
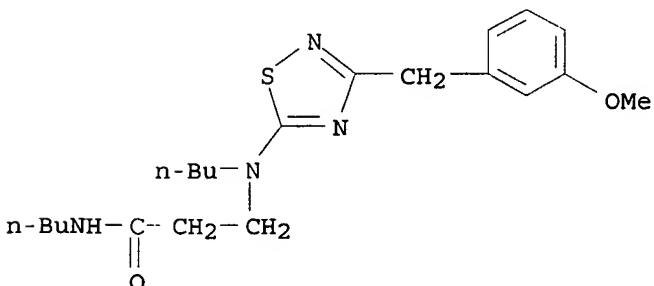LC   STN Files: CHEMCATS
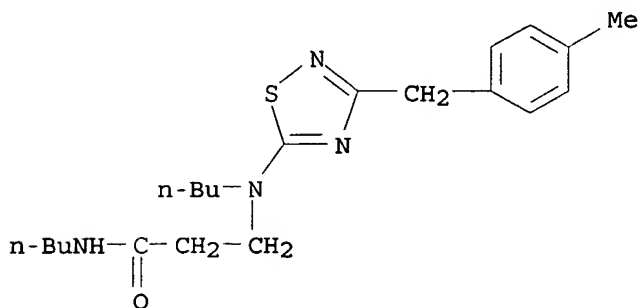
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 8 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   859346-42-2   REGISTRY
ED   Entered STN: 10 Aug 2005
CN   Propanamide, 3-[(2-methoxyethyl)[3-(phenylmethyl)-1,2,4-thiadiazol-5-
      yl]amino]-N-propyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C18 H26 N4 O2 S
SR   Chemical Library
         Supplier: ComGenex International Inc.
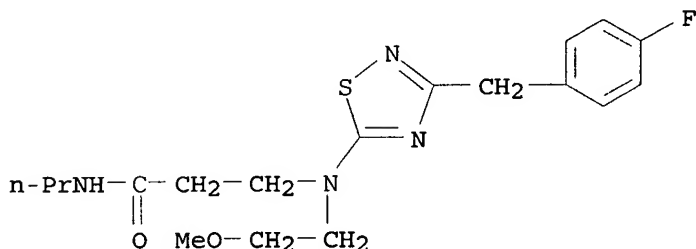LC   STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 9 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   858870-62-9   REGISTRY
ED   Entered STN: 08 Aug 2005
CN   Propanamide, N-butyl-3-[butyl[3-[(3-methoxyphenyl)methyl]-1,2,4-thiadiazol-
      5-yl]amino]- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
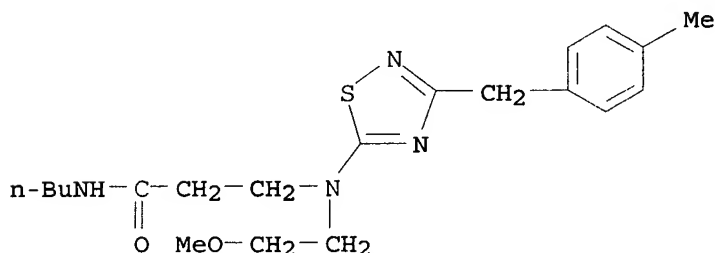MF   C21 H32 N4 O2 S
SR   Chemical Library

L3   ANSWER 10 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   858073-56-0   REGISTRY
ED   Entered STN: 03 Aug 2005
CN   Propanamide, 3-[[3-[(4-fluorophenyl)methyl]-1,2,4-thiadiazol-5-yl](2-
      methoxyethyl)amino]-N-propyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C18 H25 F N4 O2 S
SR   Chemical Library

L3   ANSWER 11 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   857863-50-4   REGISTRY
ED   Entered STN: 01 Aug 2005
CN   Propanamide, N-butyl-3-[(2-methoxyethyl)[3-[(4-methylphenyl)methyl]-1,2,4-
      thiadiazol-5-yl]amino]- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C20 H30 N4 O2 S
SR   Chemical Library
         Supplier: ComGenex International Inc.
LC   STN Files: CHEMCATS

L3   ANSWER 12 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   857313-99-6   REGISTRY
ED   Entered STN: 27 Jul 2005
CN   Acetamide, N-butyl-2-[[4-chloro-6-[[2-(dimethylamino)ethyl](phenylmethyl)a
      mino]-2-pyrimidinyl]thio]- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C21 H30 Cl N5 O S
SR   Chemical Library

n-BuNH—C(=O)—CH$_2$—S

O (double bond on C)

Cl (on pyrimidine ring), N—CH$_2$—CH$_2$—NMe$_2$, CH$_2$—Ph
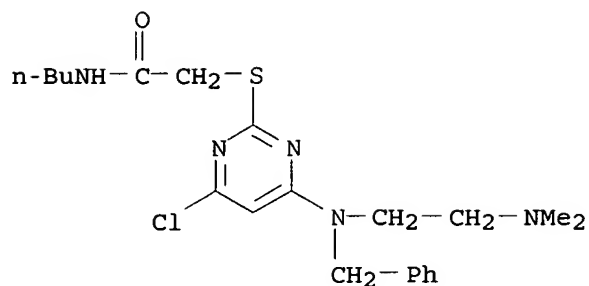
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 13 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   855131-73-6   REGISTRY
ED   Entered STN: 14 Jul 2005
CN   Propanamide, 3-[butyl[3-[(3-methoxyphenyl)methyl]-1,2,4-thiadiazol-5-
      yl]amino]-N-propyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C20 H30 N4 O2 S
SR   Chemical Library
         Supplier: ComGenex International Inc.
LC   STN Files: CHEMCATS
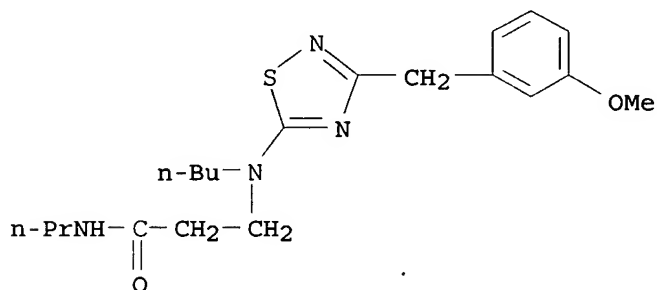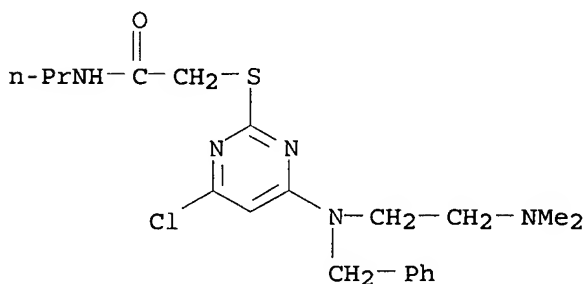
CH$_2$— OMe

n-Bu—N

n-PrNH—C—CH$_2$—CH$_2$

O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 14 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   854537-47-6   REGISTRY
ED   Entered STN: 11 Jul 2005
CN   Acetamide, 2-[[4-chloro-6-[[2-(dimethylamino)ethyl](phenylmethyl)amino]-2-
      pyrimidinyl]thio]-N-propyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C20 H28 Cl N5 O S
SR   Chemical Library
         Supplier: ComGenex International Inc.
LC   STN Files: CHEMCATS

O

n-PrNH—C—CH$_2$—S

Cl, N—CH$_2$—CH$_2$—NMe$_2$, CH$_2$—Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 15 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   854330-82-8   REGISTRY
ED   Entered STN: 10 Jul 2005
CN   Propanamide, 3-[butyl[3-[(4-methylphenyl)methyl]-1,2,4-thiadiazol-5-
      yl]amino]-N-propyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C20 H30 N4 O S
SR   Chemical Library
         Supplier: ComGenex International Inc.
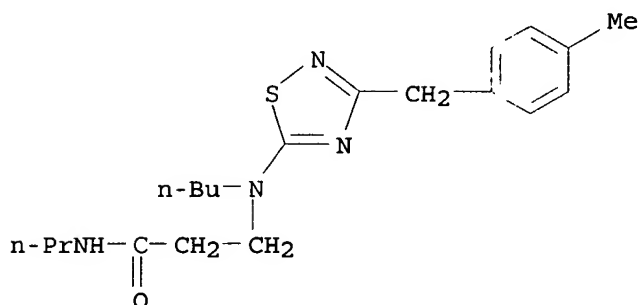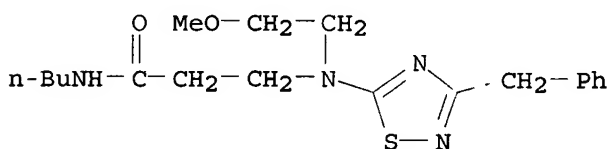LC   STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 16 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   853702-15-5   REGISTRY
ED   Entered STN: 04 Jul 2005
CN   Propanamide, N-butyl-3-[(2-methoxyethyl)[3-(phenylmethyl)-1,2,4-thiadiazol-
      5-yl]amino]- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C19 H28 N4 O2 S
SR   Chemical Library
         Supplier: ComGenex International Inc.
LC   STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT
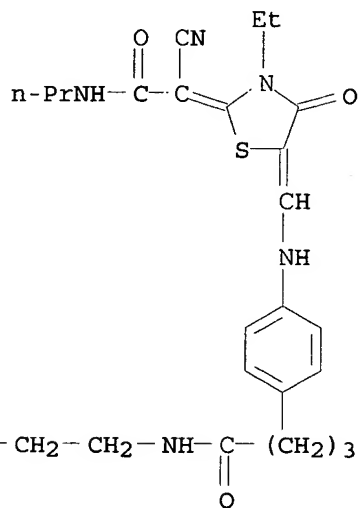

L3   ANSWER 17 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   853302-77-9   REGISTRY
ED   Entered STN: 30 Jun 2005
CN   2-Quinazolineacetamide, α-[(4-bromobenzoyl)[3-
      (dimethylamino)propyl]amino]-7-chloro-N-ethyl-3,4-dihydro-4-oxo-3-
      (phenylmethyl)- (9CI)   (CA INDEX NAME)
MF   C31 H33 Br Cl N5 O3
SR   CA
LC   STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
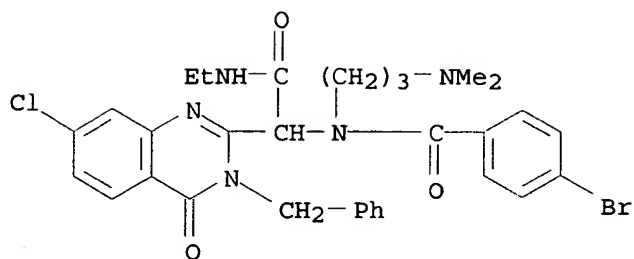
Structure 1

EtNH—C(=O)—C(CH₂)₃—NMe₂ ... CH—N—C(=O)—(4-Br-C₆H₄)

Structure: 7-Cl quinazolin-4-one with 3-(CH₂—Ph), 2-CH linked to N

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

                    1 REFERENCES IN FILE CA (1907 TO DATE)
                    1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3	ANSWER 18 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN	851651-32-6 REGISTRY
ED	Entered STN: 03 Jun 2005
CN	Benzenebutanamide, 4-[[[2-[1-cyano-2-oxo-2-(propylamino)ethylidene]-3-ethyl-4-oxo-5-thiazolidinylidene]methyl]amino]-N-[2-(diethylamino)ethyl]-(9CI) (CA INDEX NAME)
FS	3D CONCORD
MF	C28 H40 N6 O3 S
SR	CA
LC	STN Files: CA, CAPLUS, TOXCENTER

Structure 2

n-PrNH—C(=O)—C(CN)= thiazolidinone with N—Et, =O, S, =CH—NH—(aryl)

Et₂N—CH₂—CH₂—NH—C(=O)—(CH₂)₃

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

                    1 REFERENCES IN FILE CA (1907 TO DATE)
                    1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3	ANSWER 19 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN	851649-20-2 REGISTRY
ED	Entered STN: 03 Jun 2005
CN	1H-Indole-3-carboxamide, 5-[[[2-[1-cyano-2-(ethylamino)-2-oxoethylidene]-3-ethyl-4-oxo-5-thiazolidinylidene]methyl]amino]-N-[2-(dimethylamino)ethyl]-N-methyl- (9CI) (CA INDEX NAME)
FS	3D CONCORD
MF	C25 H31 N7 O3 S
SR	CA
LC	STN Files: CA, CAPLUS, TOXCENTER

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

      1 REFERENCES IN FILE CA (1907 TO DATE)
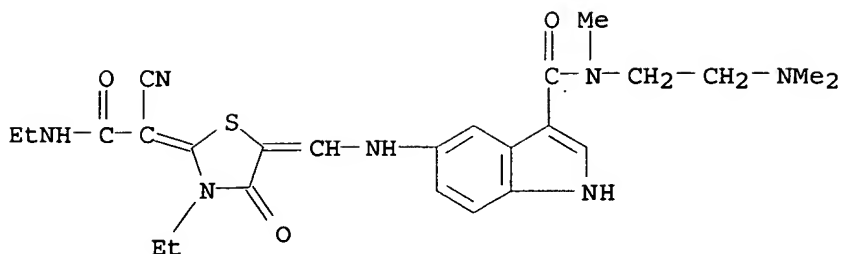   1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 20 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN   851649-16-6 REGISTRY
ED   Entered STN: 03 Jun 2005
CN   1H-Indole-3-carboxamide, 6-[[[2-[1-cyano-2-(ethylamino)-2-oxoethylidene]-3-
      ethyl-4-oxo-5-thiazolidinylidene]methyl]amino]-N-[2-(dimethylamino)ethyl]-
      (9CI) (CA INDEX NAME)
FS   3D CONCORD
MF   C24 H29 N7 O3 S
SR   CA
LC   STN Files: CA, CAPLUS, TOXCENTER

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

      1 REFERENCES IN FILE CA (1907 TO DATE)
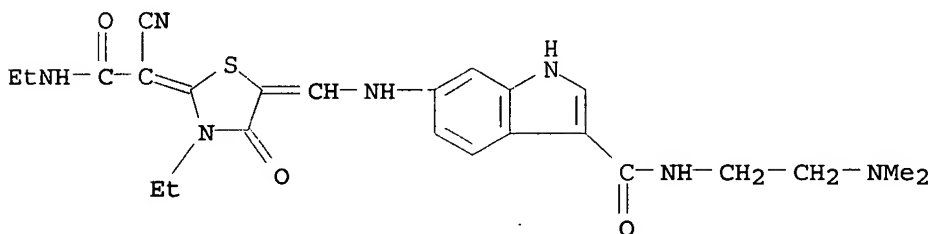   1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

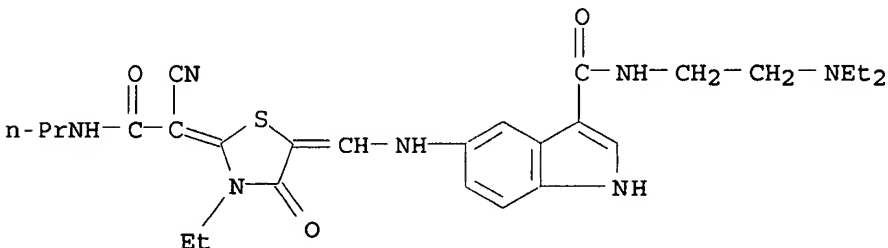L3   ANSWER 21 OF 48 REGISTRY COPYRIGHT 2006 ACS on STN
RN   851649-08-6 REGISTRY
ED   Entered STN: 03 Jun 2005
CN   1H-Indole-3-carboxamide, 5-[[[2-[1-cyano-2-oxo-2-(propylamino)ethylidene]-
      3-ethyl-4-oxo-5-thiazolidinylidene]methyl]amino]-N-[2-(diethylamino)ethyl]-
      (9CI) (CA INDEX NAME)
FS   3D CONCORD
MF   C27 H35 N7 O3 S
SR   CA
LC   STN Files: CA, CAPLUS, TOXCENTER

L3   ANSWER 22 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   832083-67-7   REGISTRY
ED   Entered STN: 16 Feb 2005
CN   3-Pyrrolidineacetamide, 1-[4-[4-[[1-[(2,6-dimethoxyphenyl)methyl]-4-
       piperidinyl]methylamino]butoxy]butyl]-N-methyl-α,α-diphenyl-,
       (3S)- (9CI)   (CA INDEX NAME)
OTHER NAMES:
CN   (S)-4-[N-[9-[3-[1-(Methylcarbamoyl)-1,1-diphenylmethyl]pyrrolidin-1-yl]-5-
       oxanon-1-yl]-N-(methyl)amino]-1-(2,6-dimethoxybenzyl)piperidine
FS   STEREOSEARCH
MF   C42 H60 N4 O4
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

L3   ANSWER 23 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   832083-61-1   REGISTRY
ED   Entered STN: 16 Feb 2005
CN   3-Pyrrolidineacetamide, 1-[7-[[1-[(2,6-dimethoxyphenyl)methyl]-4-
       piperidinyl](1-methylethyl)amino]heptyl]-N-methyl-α,α-diphenyl-
       , (3S)- (9CI)   (CA INDEX NAME)
OTHER NAMES:
CN   (S)-4-[N-[7-[3-[1-(Methylcarbamoyl)-1,1-diphenylmethyl]pyrrolidin-1-
       yl]hept-1-yl]-N-(isopropyl)amino]-1-(2,6-dimethoxybenzyl)piperidine
FS   STEREOSEARCH
MF   C43 H62 N4 O3
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

L3   ANSWER 24 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   832083-27-9   REGISTRY
ED   Entered STN: 16 Feb 2005
CN   3-Pyrrolidineacetamide, 1-[7-[(cyclopropylmethyl)[1-[(2,6-
        dimethoxyphenyl)methyl]-4-piperidinyl]amino]heptyl]-N-methyl-
        α,α-diphenyl-, (3S)- (9CI)   (CA INDEX NAME)
OTHER NAMES:
CN   (S)-4-[N-[7-[3-[1-(Methylcarbamoyl)-1,1-diphenylmethyl]pyrrolidin-1-
        yl]hept-1-yl]-N-(cyclopropylmethyl)amino]-1-(2,6-
        dimethoxybenzyl)piperidine
FS   STEREOSEARCH
MF   C44 H62 N4 O3
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

L3   ANSWER 25 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   832083-24-6   REGISTRY
ED   Entered STN: 16 Feb 2005
CN   3-Pyrrolidineacetamide, 1-[9-[[1-[(2,6-dimethoxyphenyl)methyl]-4-
        piperidinyl]methylamino]nonyl]-N-methyl-α,α-diphenyl-, (3S)-
        (9CI)   (CA INDEX NAME)
OTHER NAMES:
CN   (S)-4-[N-[9-[3-[1-(Methylcarbamoyl)-1,1-diphenylmethyl]pyrrolidin-1-yl]non-

1-yl]-N-(methyl)amino]-1-(2,6-dimethoxybenzyl)piperidine
FS   STEREOSEARCH
MF   C43 H62 N4 O3
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL
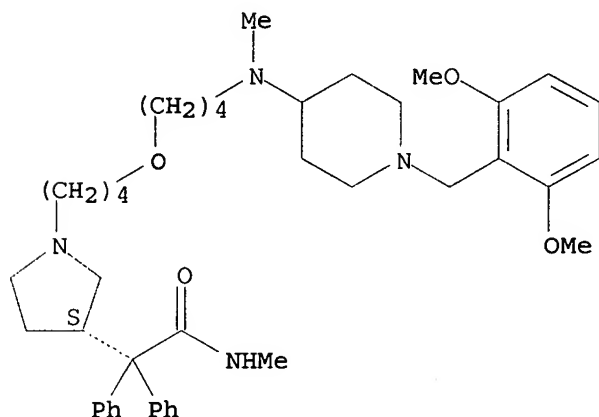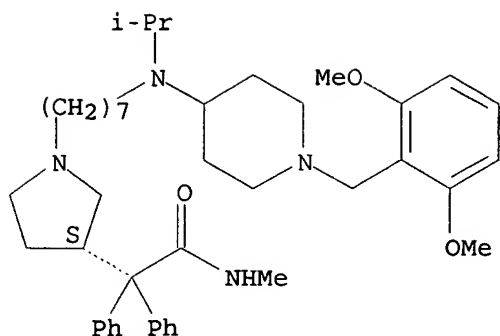
Absolute stereochemistry.
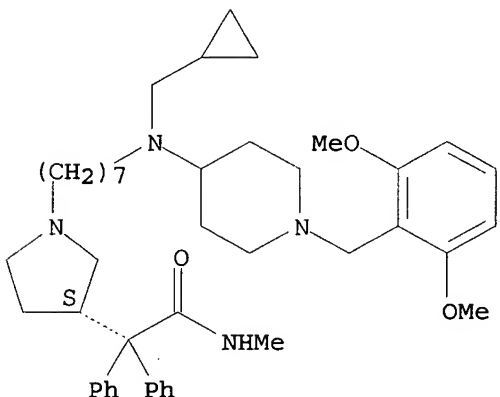

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

              1 REFERENCES IN FILE CA (1907 TO DATE)
              1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 26 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   832082-50-5   REGISTRY
ED   Entered STN: 16 Feb 2005
CN   3-Pyrrolidineacetamide, 1-[7-[[1-[(2,6-dimethoxyphenyl)methyl]-4-
      piperidinyl]propylamino]heptyl]-N-methyl-α,α-diphenyl-, (3S)-,
      mono(trifluoroacetate) (9CI)   (CA INDEX NAME)
OTHER NAMES:
CN   (S)-4-[N-[7-[3-[1-(N-Methylcarbamoyl)-1,1-diphenylmethyl]pyrrolidin-1-
      yl]hept-1-yl]-N-propylamino]-1-(2,6-dimethoxybenzyl)piperidine
      trifluoroacetate
FS   STEREOSEARCH
MF   C43 H62 N4 O3 . C2 H F3 O2
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL

      CM   1

      CRN   832082-49-2
      CMF   C43 H62 N4 O3

Absolute stereochemistry.
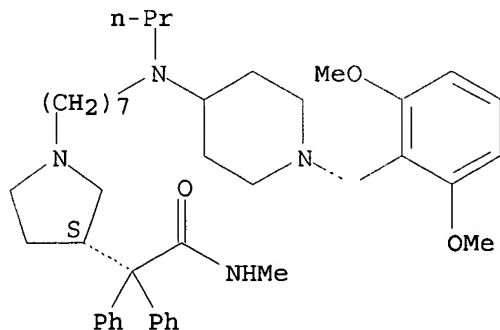
      CM   2

      CRN   76-05-1
      CMF   C2 H F3 O2
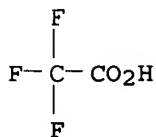
```
  F
  |
F—C—CO2H
  |
  F
```

L3   ANSWER 27 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   832082-49-2   REGISTRY
ED   Entered STN: 16 Feb 2005
CN   3-Pyrrolidineacetamide, 1-[7-[[1-[(2,6-dimethoxyphenyl)methyl]-4-
       piperidinyl]propylamino]heptyl]-N-methyl-α,α-diphenyl-, (3S)-
       (9CI) (CA INDEX NAME)
OTHER NAMES:
CN   (S)-4-[N-[7-[3-[1-(Methylcarbamoyl)-1,1-diphenylmethyl]pyrrolidin-1-
       yl]hept-1-yl]-N-(propyl)amino]-1-(2,6-dimethoxybenzyl)piperidine
FS   STEREOSEARCH
MF   C43 H62 N4 O3
CI   COM
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL
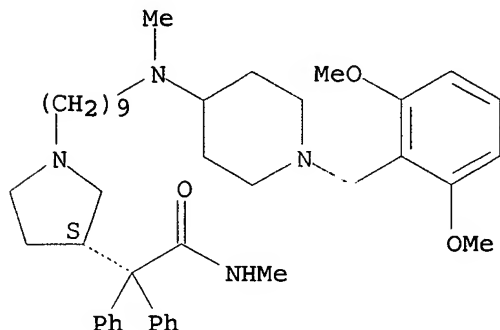
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 28 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   823817-97-6   REGISTRY
ED   Entered STN: 01 Feb 2005
CN   Carbamic acid, [(1S)-3-[bis(2-pyridinylmethyl)amino]-1-[[[(1S)-3-[bis(2-
       pyridinylmethyl)amino]-1-[(methylamino)carbonyl]propyl]amino]carbonyl]prop
       yl]-, 1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)
FS   STEREOSEARCH
MF   C38 H49 N9 O4
SR   CA
LC   STN Files: CA, CAPLUS

Absolute stereochemistry.
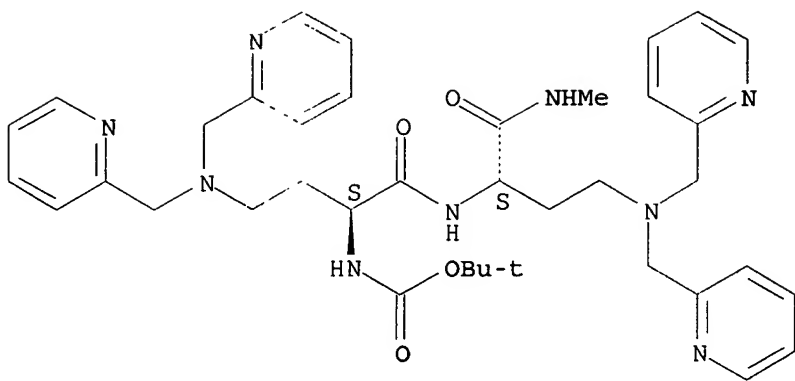
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

        1 REFERENCES IN FILE CA (1907 TO DATE)
        1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
        1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 29 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   786584-81-4 REGISTRY
ED   Entered STN: 22 Nov 2004
CN   Propanamide, 3-[[2-[(2-benzoyl-4-nitrophenyl)methylamino]-2-
      oxoethyl]butylamino]-N-butyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C27 H36 N4 O5
CI   COM
SR   CA
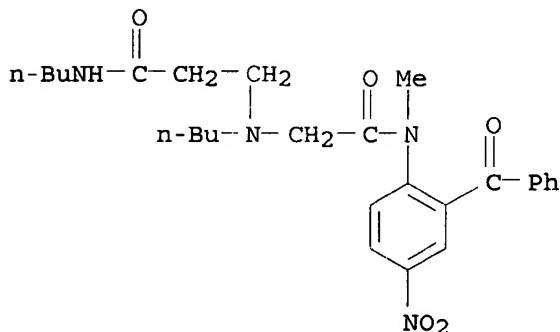
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 30 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   782469-02-7 REGISTRY
ED   Entered STN: 17 Nov 2004
CN   4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-
      tetrahydro-5-[2-methoxy-3-[3-[(5-phenylpentyl)amino]propoxy]phenyl]-2-oxo-
      N-propyl-, (3R,5S)-rel- (9CI)   (CA INDEX NAME)
FS   STEREOSEARCH
MF   C40 H54 Cl N3 O5
SR   CA
LC   STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.
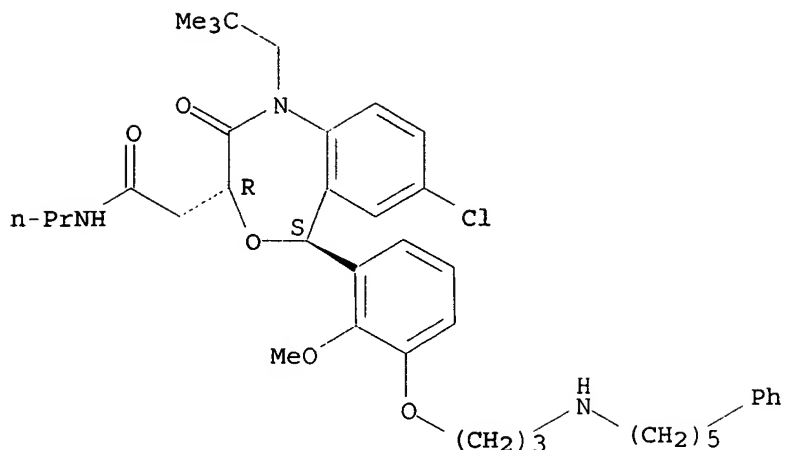
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

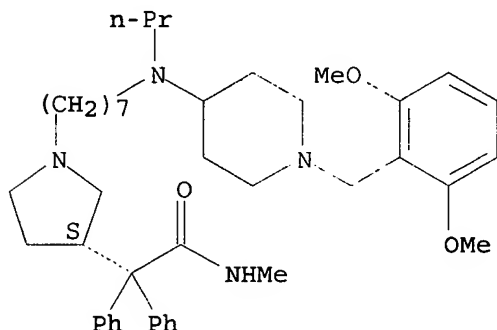   1 REFERENCES IN FILE CA (1907 TO DATE)
        1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 31 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   779993-84-9   REGISTRY
ED   Entered STN: 12 Nov 2004
CN   Benzenemethanaminium, N,N-dibutyl-N-[2-(methylamino)-2-oxoethyl]- (9CI)
       (CA INDEX NAME)
MF   C18 H31 N2 O
CI   COM
SR   CA
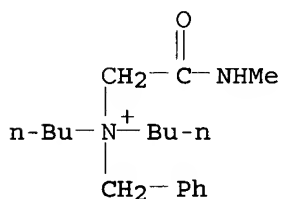
L3   ANSWER 32 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   773833-96-8   REGISTRY
ED   Entered STN: 01 Nov 2004
CN   Pentanamide, 5-[dodecyl[2-[4-(4,4,4-trifluoro-3-
       oxobutyl)phenoxy]ethyl]amino]-N-ethyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C31 H51 F3 N2 O3
CI   COM
SR   CA
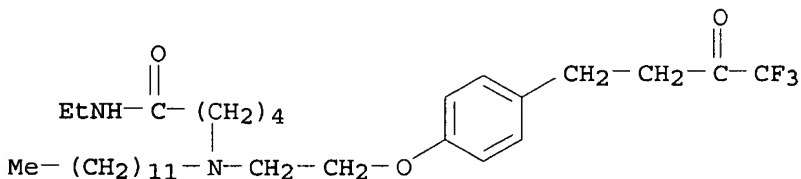
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 33 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

$$-(CH_2)_6-\underset{\underset{Me}{|}}{\overset{\overset{Me}{|}}{C}}-\Bigg]_n$$
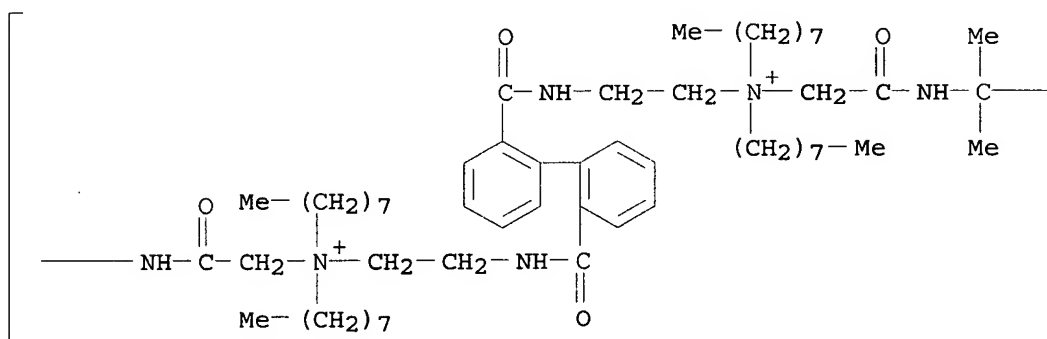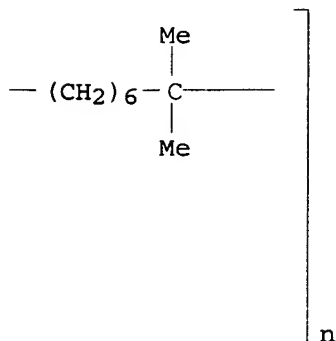
CN   Butanediamide, N1-[2-[[4-[(butylamino)carbonyl]-1-(cyclohexylmethyl)-2-
       hydroxy-5-methylhexyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-N4-[3-
       (dimethylamino)propyl]-2-(1-naphthalenylmethyl)-, [1R-[1R*[S*(S*)],3S*]]-
       (9CI)   (CA INDEX NAME)
MF   C45 H69 N7 O5
CI   COM
SR   CA

CN   Benzenepropanoic acid, β-(butylamino)-α-[2-(butylamino)-2-
       oxoethyl]-4-methoxy- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C20 H32 N2 O4
SR   CA
LC   STN Files: CA, CAPLUS
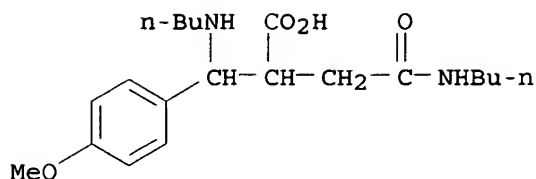
n-BuNH   CO₂H   O
  | | ||
  CH— CH— CH₂— C— NHBu-n

(structure: 4-MeO-phenyl attached to CH)

MeO—[benzene ring]—CH...

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

          1 REFERENCES IN FILE CA (1907 TO DATE)
          1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 37 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   754194-02-0   REGISTRY
ED   Entered STN: 30 Sep 2004
CN   Benzenebutanamide, N-butyl-γ-(butylamino)-β-
      (dihydroxymethylene)- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C19 H30 N2 O3
SR   CA
LC   STN Files: CA, CAPLUS
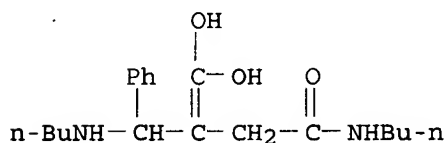
             OH
             |
      Ph   C— OH   O
      | || ||
n-BuNH— CH— C— CH₂— C— NHBu-n

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

          1 REFERENCES IN FILE CA (1907 TO DATE)
          1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 38 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   748781-96-6   REGISTRY
ED   Entered STN: 21 Sep 2004
CN   2,5,8,11-Tetraazatridecan-13-oic acid, 5,8-bis(carboxymethyl)-11-[2-
      (methylamino)-2-oxoethyl]-3-oxo-6-(phenylmethyl)-, labeled with deuterium,
      (6S)- (9CI)   (CA INDEX NAME)
FS   STEREOSEARCH
MF   C23 H27 D8 N5 O8
SR   CA
LC   STN Files: CA, CAPLUS, CASREACT
IL   8H-2

Absolute stereochemistry.

(structure: tetraaza compound with CO₂H, Ph, MeNH, NHMe, HO₂C, CO₂H groups, S configuration)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

          1 REFERENCES IN FILE CA (1907 TO DATE)
          1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

RN   748781-95-5   REGISTRY
ED   Entered STN: 21 Sep 2004
CN   2,5,8,11-Tetraazatridecan-13-oic acid, 5,8-bis(carboxymethyl)-6-[(4-
       ethoxyphenyl)methyl]-11-[2-(methylamino)-2-oxoethyl]-3-oxo-, labeled with
       deuterium, (6S)- (9CI)   (CA INDEX NAME)
FS   STEREOSEARCH
MF   C25 H31 D8 N5 O9
SR   CA
LC   STN Files: CA, CAPLUS, CASREACT
IL   8H-2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

            1 REFERENCES IN FILE CA (1907 TO DATE)
            1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

RN   748781-94-4   REGISTRY
ED   Entered STN: 21 Sep 2004
CN   2,5,8,11-Tetraazatridecan-13-oic acid, 5,8-bis(carboxymethyl)-11-[2-
       (methylamino)-2-oxoethyl]-3-oxo-6-(phenylmethyl)-, (6S)- (9CI)   (CA INDEX
       NAME)
FS   STEREOSEARCH
MF   C23 H35 N5 O8
SR   CA
LC   STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

            1 REFERENCES IN FILE CA (1907 TO DATE)
            1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

RN   748781-93-3   REGISTRY
ED   Entered STN: 21 Sep 2004
CN   2,5,8,11-Tetraazatridecan-13-oic acid, 5,8-bis(carboxymethyl)-6-[(4-

ethoxyphenyl)methyl]-11-[2-(methylamino)-2-oxoethyl]-3-oxo-, (6S)- (9CI)
(CA INDEX NAME)
FS   STEREOSEARCH
MF   C25 H39 N5 O9
SR   CA
LC   STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

        1 REFERENCES IN FILE CA (1907 TO DATE)
        1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 42 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   738527-69-0   REGISTRY
ED   Entered STN: 03 Sep 2004
CN   Propanamide, N-(2-benzoyl-4-chlorophenyl)-2-[butyl[3-(butylamino)-3-
      oxopropyl]amino]-N-methyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C28 H38 Cl N3 O3
CI   COM
SR   CA

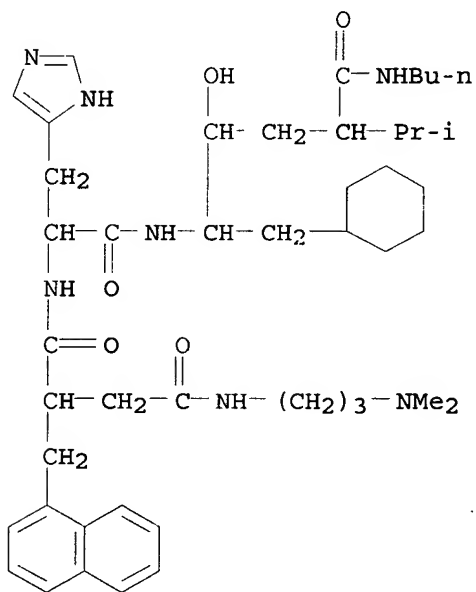**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L3   ANSWER 43 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   736907-02-1   REGISTRY
ED   Entered STN: 01 Sep 2004
CN   L-Leucinamide, N-methyl-N-[1-oxo-2,6-bis(trimethylammonio)hexyl]glycyl-N-
      methylglycyl-N-methyl-L-phenylalanyl-N,N2-dimethyl-, (S)- (9CI)   (CA INDEX
      NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
MF   C36 H65 N7 O5
CI   COM
SR   CA

Absolute stereochemistry.
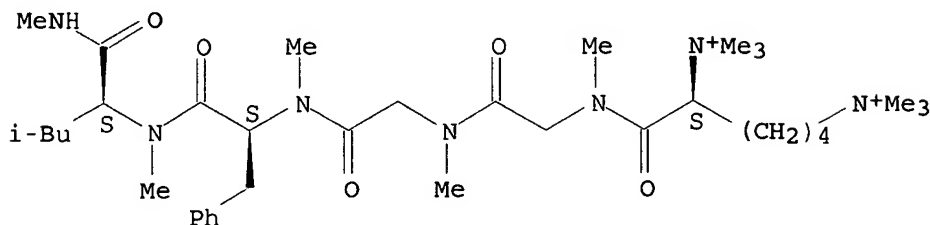
L3   ANSWER 44 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   735251-98-6   REGISTRY
ED   Entered STN: 29 Aug 2004
CN   Butanamide, 4-[dodecyl[2-[4-(4,4,4-trifluoro-3-
        oxobutyl)phenoxy]ethyl]amino]-N-ethyl- (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C30 H49 F3 N2 O3
CI   COM
SR   CA
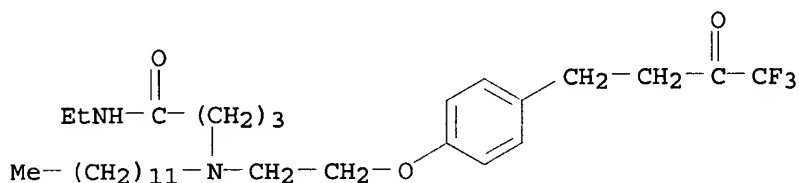
L3   ANSWER 45 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   697215-05-7   REGISTRY
ED   Entered STN: 21 Jun 2004
CN   Benzeneacetic acid, α-[(ethylamino)carbonyl]-, 2-(diethylamino)ethyl
        ester (9CI)   (CA INDEX NAME)
FS   3D CONCORD
MF   C17 H26 N2 O3
CI   COM
SR   CA
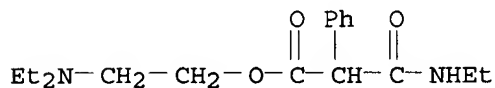
L3   ANSWER 46 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   691000-68-7   REGISTRY
ED   Entered STN: 09 Jun 2004
CN   3-Pyrrolidineacetamide, 1-[7-[[1-[(4-methoxy-3-pyridinyl)methyl]-4-
        piperidinyl](1-methylethyl)amino]heptyl]-N-methyl-α,α-diphenyl-
        , (3S)- (9CI)   (CA INDEX NAME)
OTHER NAMES:
CN   (S)-4-[N-[7-[3-[(Methylcarbamoyl)diphenylmethyl]pyrrolidin-1-yl]hept-1-yl]-
        N-(isopropyl)amino]-1-[(4-methoxypyridin-3-yl)methyl]piperidine

Absolute stereochemistry.

i-Pr

(CH₂)₇ N
        N   MeO
                                     N
(CH₂)₇
N
        S
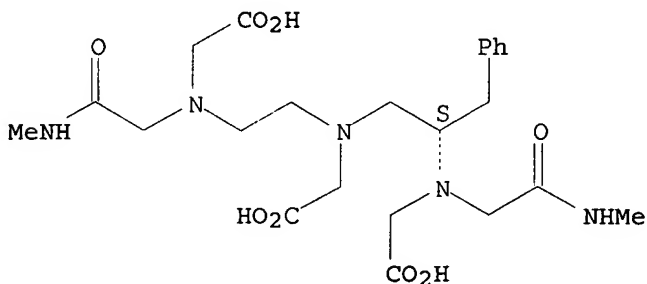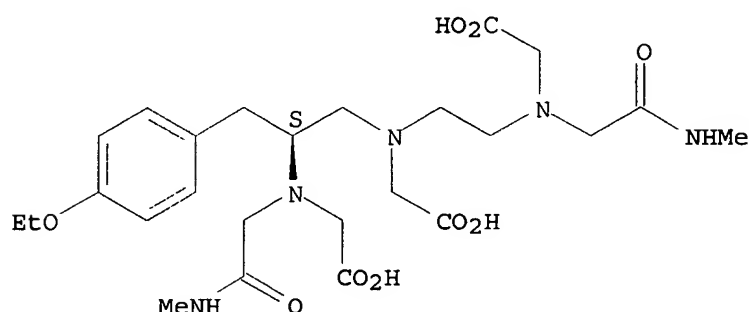   O
                   NHMe
Ph Ph
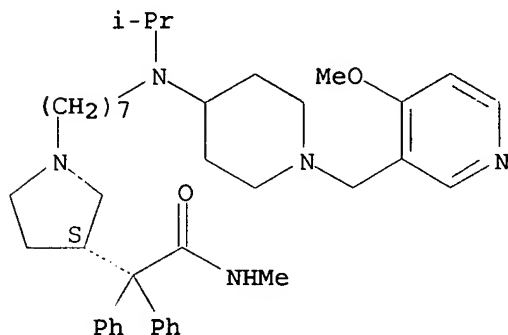
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3   ANSWER 47 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   690952-92-2 REGISTRY
ED   Entered STN: 08 Jun 2004
CN   Benzenepropanamide, N-butyl-α-[(2S,3S)-4-cyclohexyl-2-hydroxy-3-[(4-
      methylpentyl)amino]butyl]-, (αR)- (9CI)   (CA INDEX NAME)
FS   STEREOSEARCH
MF   C29 H50 N2 O2
CI   COM
SR   CA

Absolute stereochemistry.

                   Ph

         OH
              S   S   R   NHBu-n
                                     O
         HN
              (CH₂)₃   CHMe₂
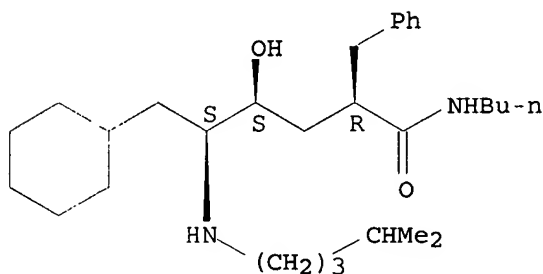
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   ANSWER 48 OF 48   REGISTRY   COPYRIGHT 2006 ACS on STN
RN   687620-30-0 REGISTRY
ED   Entered STN: 31 May 2004
CN   Butanediamide, N1-[(1S)-2-[[(1S,2S,4S)-4-[(butylamino)carbonyl]-1-
      (cyclohexylmethyl)-2-hydroxy-5-methylhexyl]amino]-1-(1H-imidazol-4-
      ylmethyl)-2-oxoethyl]-N4-[3-(dimethylamino)propyl]-2-(1-
      naphthalenylmethyl)-, (2S)- (9CI)   (CA INDEX NAME)
MF   C45 H69 N7 O5
CI   COM
SR   CA

```
      N═
    ╱     ╲           OH            O
   N        NH                      ‖
    ╲     ╱           │             C─NHBu-n
                      CH─CH₂─CH─Pr-i │
   CH2                              CH─CH₂─CH─Pr-i
    │
   CH─C─NH─CH─CH₂─⬡
    │  ‖
   NH  O
    │
   C═O        O
    │         ‖
   CH─CH₂─C─NH─(CH₂)₃─NMe₂
    │
   CH2
    │
   (naphthalene)
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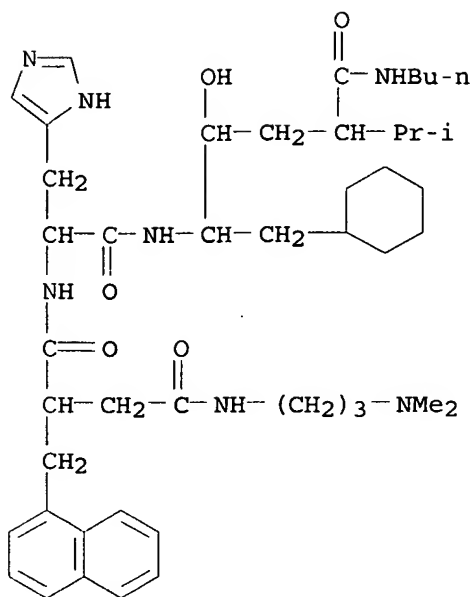
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COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                 ENTRY   SESSION
FULL ESTIMATED COST   259.46   259.67

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FILE LAST UPDATED: 29 Jan 2006   (20060129/ED)

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L4   12 L3

=> d l4 1-12

L4   ANSWER 1 OF 12   CAPLUS   COPYRIGHT 2006 ACS on STN
AN   2005:1005977   CAPLUS
DN   143:306185
TI   Preparation of biphenyl compounds useful as muscarinic receptor
      antagonists
IN   Mammen, Mathai; Ji, Yu-Hua; Mu, Yongqi; Malathong, Viengkham
PA   Theravance, Inc., USA
SO   U.S. Pat. Appl. Publ., 48 pp.
      CODEN: USXXCO
DT   Patent

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LA      English
FAN.CNT 1
        PATENT NO.              KIND   DATE      APPLICATION NO.            DATE
        ---------------         ----   --------  --------------------      --------
PI  US 2005203083               A1     20050915  US 2005-77224             20050310
    WO 2005087732               A1     20050922  WO 2005-US7987            20050310
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            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
            SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
            RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
            MR, NE, SN, TD, TG
PRAI US 2004-552421P            P      20040311
OS  MARPAT 143:306185


L4  ANSWER 2 OF 12   CAPLUS   COPYRIGHT 2006 ACS on STN
AN  2005:1004718  CAPLUS
DN  143:306311
TI  Preparation of N-arylmethyl or N-heterocyclylmethyl-N-(imidazol-2-
    ymethyl)amines as antagonists of chemokine receptor CXCR4
IN  Saitou, Atsushi; Kikumoto, Shigeyuki; Ono, Masahiro; Matsui, Ryo;
    Yamamoto, Masashi; Sawa, Tomohiro; Suzuki, Shigeru; Yanaka, Mikiro
PA  Kureha Chemical Industry Company, Limited, Japan
SO  PCT Int. Appl., 252 pp.
    CODEN: PIXXD2
DT  Patent
LA  Japanese
FAN.CNT 1
        PATENT NO.              KIND   DATE       APPLICATION NO.           DATE
        ---------------         ----   --------   --------------------      --------
PI  WO 2005085209               A1     20050915   WO 2005-JP4189            20050310
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
            SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
            RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
            MR, NE, SN, TD, TG
PRAI JP 2004-68229              A      20040310
     JP 2004-350599             A      20041203
OS  MARPAT 143:306311
RE.CNT  15      THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT


L4  ANSWER 3 OF 12   CAPLUS   COPYRIGHT 2006 ACS on STN
AN  2005:823706  CAPLUS
DN  143:211891
TI  Preparation of diazanaphthalene derivatives as HIV integrase inhibitors
IN  Taishi, Teruhiko; Tada, Yukio
PA  Shionogi & Co., Ltd., Japan
SO  PCT Int. Appl., 79 pp.
    CODEN: PIXXD2
DT  Patent
LA  Japanese
FAN.CNT 1
        PATENT NO.              KIND   DATE       APPLICATION NO.           DATE
        ---------------         ----   --------   --------------------      --------
PI  WO 2005075475               A1     20050818   WO 2005-JP1454            20050202
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
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              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
              RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
              MR, NE, SN, TD, TG
PRAI JP 2004-27849       A      20040204
OS   MARPAT 143:211891
RE.CNT 13      THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
               ALL CITATIONS AVAILABLE IN THE RE FORMAT


L4   ANSWER 4 OF 12  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2005:559569  CAPLUS
DN   143:230177
TI   Iterative Approach to the Discovery of Novel Degarelix Analogues:
     Substitutions at Positions 3, 7, and 8. Part II
AU   Samant, Manoj P.; Gulyas, Jozsef; Hong, Doley J.; Croston, Glenn; Rivier,
     Catherine; Rivier, Jean
CS   Clayton Foundation Laboratories for Peptide Biology, The Salk Institute
     for Biological Studies, La Jolla, CA, 92037, USA
SO   Journal of Medicinal Chemistry (2005), 48(15), 4851-4860
     CODEN: JMCMAR; ISSN: 0022-2623
PB   American Chemical Society
DT   Journal
LA   English
OS   CASREACT 143:230177
RE.CNT 56      THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
               ALL CITATIONS AVAILABLE IN THE RE FORMAT


L4   ANSWER 5 OF 12  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2005:490357  CAPLUS
DN   143:43896
TI   Preparation of quinazolinone compounds as anticancer agents
IN   Wang, Weibo; Lagniton, Liana M.; Constantine, Ryan N.; Desai, Manoj C.
PA   Chiron Corporation, USA
SO   PCT Int. Appl., 64 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE      APPLICATION NO.         DATE
     ---------------     ----   --------  --------------------    --------
PI   WO 2005051922       A1     20050609  WO 2004-US39448         20041124
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO,
             SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
     US 2005209254       A1     20050922  US 2004-996814          20041124
PRAI US 2003-525059P     P      20031125
OS   MARPAT 143:43896
RE.CNT 3       THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
               ALL CITATIONS AVAILABLE IN THE RE FORMAT


L4   ANSWER 6 OF 12  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2005:409495  CAPLUS
DN   142:463714
TI   Preparation of thiazolidinones as polo like kinase (PLK) inhibitors
IN   Schulze, Volker; Eis, Knut; Wortmann, Lars; Schwede, Wolfgang; Siemeister,
     Gerhard; Briem, Hans; Schneider, Herbert; Eberspaecher, Uwe; Hess-Stumpp,
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        Holger
PA      Schering Aktiengesellschaft, Germany
SO      PCT Int. Appl., 326 pp.
        CODEN: PIXXD2
DT      Patent
LA      German
FAN.CNT 1
        PATENT NO.             KIND   DATE        APPLICATION NO.          DATE
        ---------------        ----   --------    --------------------     --------
PI   WO 2005042505             A1     20050512    WO 2004-EP12242           20041026
        W:   AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW:  BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
        DE 10351744            A1     20050616    DE 2003-10351744          20031031
PRAI DE 2003-10351744          A      20031031
OS      MARPAT 142:463714
RE.CNT  2       THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT


L4      ANSWER 7 OF 12   CAPLUS   COPYRIGHT 2006 ACS on STN
AN      2005:74113   CAPLUS
DN      142:176696
TI      Preparation of substituted 4-amino-1-benzylpiperidines as muscarinic M2
        receptor antagonists
IN      Mammen, Mathai; Wilson, Richard; Dunham, Sarah; Hughes, Adam; Husfeld,
        Craig; Ji, Yu-Hua; Li, Li; Mischki, Trevor; Stergiades, Ioanna; Oare,
        David
PA      Theravance, Inc., USA
SO      PCT Int. Appl., 139 pp.
        CODEN: PIXXD2
DT      Patent
LA      English
FAN.CNT 1
        PATENT NO.             KIND   DATE        APPLICATION NO.          DATE
        ---------------        ----   --------    --------------------     --------
PI   WO 2005007645             A1     20050127    WO 2004-US22264           20040709
        W:   AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW:  BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
        US 2005026954          A1     20050203    US 2004-888855            20040709
PRAI US 2003-486337P           P      20030711
OS      MARPAT 142:176696
RE.CNT  4       THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT


L4      ANSWER 8 OF 12   CAPLUS   COPYRIGHT 2006 ACS on STN
AN      2004:902194   CAPLUS
DN      141:395590
TI      Preparation of benzoxazepine compounds as RFRP receptor antagonists
IN      Itoh, Fumio; Hinuma, Shuji; Kanzaki, Naoyuki; Mabuchi, Hiroshi; Yoshida,
        Hiromi; Matsumoto, Hirokazu; Wakabayashi, Takeshi
PA      Takeda Chemical Industries Ltd., Japan
SO      PCT Int. Appl., 226 pp.
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        CODEN: PIXXD2
DT      Patent
LA      Japanese
FAN.CNT 1
        PATENT NO.            KIND    DATE         APPLICATION NO.            DATE
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PI   WO 2004091628            A1      20041028     WO 2004-JP5406            20040415
         W:   AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW:  BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
              BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
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              SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
              TD, TG
     JP 2004331659            A2      20041125     JP 2004-120246            20040415
PRAI JP 2003-114313           A       20030418
OS   MARPAT 141:395590
RE.CNT  23      THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT


L4   ANSWER 9 OF 12  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2004:412935  CAPLUS
DN   140:423591
TI   Preparation of substituted 4-amino-1-(pyridylmethyl)piperidine and related
     compounds as muscarinic receptor antagonists
IN   Mammen, Mathai; Wilson, Richard; Chen, Yan; Dunham, Sarah; Hughes, Adam;
     Husfeld, Craig; Ji, Yu-Hua; Li, Li; Mischki, Trevor; Stergiades, Ioanna
PA   Theravance, Inc., USA
SO   PCT Int. Appl., 129 pp.
        CODEN: PIXXD2
DT      Patent
LA      English
FAN.CNT 1
        PATENT NO.            KIND    DATE         APPLICATION NO.            DATE
        --------------        ----    --------     --------------------      --------
PI   WO 2004041806            A2      20040521     WO 2003-US34444           20031029
     WO 2004041806            A3      20040805
         W:   AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
              CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
              GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
              LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
              OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
              TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW:  GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
              KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
              FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
              BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2500800               AA      20040521     CA 2003-2500800           20031029
     US 2004122014            A1      20040624     US 2003-696464            20031029
     EP 1556372               A2      20050727     EP 2003-779416            20031029
         R:   AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     BR 2003015778            A       20050906     BR 2003-15778             20031029
     NO 2005002521            A       20050525     NO 2005-2521              20050525
PRAI US 2002-422229P          P       20021030
     US 2003-486483P          P       20030711
     WO 2003-US34444          W       20031029
OS   MARPAT 140:423591


L4   ANSWER 10 OF 12  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2004:314220  CAPLUS
DN   142:114408
TI   Dipeptide-based dinuclear Zn(II) complexes promoting phosphodiester bond
     cleavage
AU   Sakai, Nobue; Izuhara, Nobuko; Yamamura, Hatsuo; Kawai, Masao
```

CS   Graduate School of Engineering, Nagoya Institute of Technology, Nagoya,
      466-8555, Japan
SO   Peptide Science (2003), Volume Date 2004, 40th, 333-334
      CODEN: PSCIFQ; ISSN: 1344-7661
PB   Japanese Peptide Society
DT   Journal
LA   English
RE.CNT   2   THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4   ANSWER 11 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
AN   2004:161046   CAPLUS
DN   141:260309
TI   Factors affecting condensation of γ-phenyl and γ-(p-
      methoxyphenyl) itaconic anhydrides with different hydrazines and amines.
      Study of the antimicrobial activity of some of the products
AU   Abdel Wahhab, Samiha M.; Abdallah, Shadia M.; Elmaria, Fatma A.; Mansour,
      Eman A.; Awad, Hassan M.
CS   Chemistry Department, Faculty of Girls for Arts, Science and Education,
      Ain Shams University, Cairo, Egypt
SO   Revue Roumaine de Chimie (2003), 48(8), 619-627
      CODEN: RRCHAX; ISSN: 0035-3930
PB   Editura Academiei Romane
DT   Journal
LA   English
RE.CNT   6   THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4   ANSWER 12 OF 12 CAPLUS COPYRIGHT 2006 ACS on STN
AN   2004:156419   CAPLUS
DN   141:235023
TI   New bifunctional contrast agents: Bis-amide derivatives of C-substituted
      Gd-DTPA
AU   Laurent, Sophie; Botteman, Francois; Vander Elst, Luce; Muller, Robert N.
CS   NMR Laboratory, Department of Organic Chemistry, University of
      Mons-Hainaut, Mons, 7000, Belg.
SO   European Journal of Inorganic Chemistry (2004), (3), 463-468
      CODEN: EJICFO; ISSN: 1434-1948
PB   Wiley-VCH Verlag GmbH & Co. KGaA
DT   Journal
LA   English
OS   CASREACT 141:235023
RE.CNT   16   THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT

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                                                    ENTRY        SESSION
FULL ESTIMATED COST                                  0.21          0.21

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DICTIONARY FILE UPDATES:  29 JAN 2006   HIGHEST RN 872967-60-7

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* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

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for details.

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
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L1        STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1                STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 10:10:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    91532 TO ITERATE

  2.2% PROCESSED     2000 ITERATIONS                        0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
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FULL FILE PROJECTIONS:    ONLINE   **INCOMPLETE**
                          BATCH    **INCOMPLETE**
PROJECTED ITERATIONS:       1812685 TO   1848595
PROJECTED ANSWERS:                0 TO         0


L2              0 SEA SSS SAM L1

=>
Uploading C:\Program Files\Stnexp\Queries\08791.str

L3        STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3                 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l3
SAMPLE SEARCH INITIATED 10:12:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    31679 TO ITERATE

  6.3% PROCESSED      2000 ITERATIONS                        0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE   **COMPLETE**
                          BATCH    **COMPLETE**
PROJECTED ITERATIONS:        622941 TO    644219
PROJECTED ANSWERS:                0 TO         0


L4              0 SEA SSS SAM L3

=> s l3 ful
FULL SEARCH INITIATED 10:13:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   634690 TO ITERATE

100.0% PROCESSED   634690 ITERATIONS                        0 ANSWERS
SEARCH TIME: 00.00.04

L5              0 SEA SSS FUL L3
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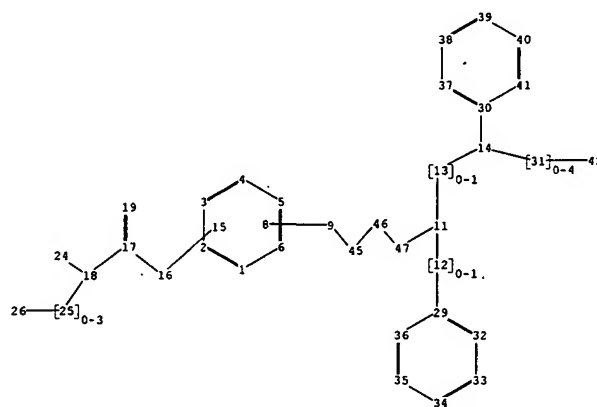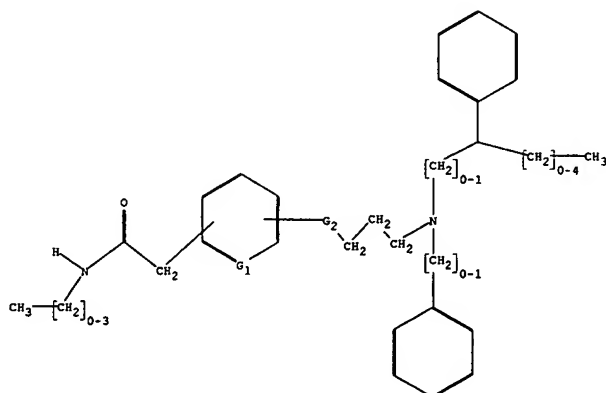
chain nodes :
    8   9   11   12   13   14   15   16   17   18   19   24   25   26   31   42   45   46   47
ring nodes :
    1   2   3   4   5   6   29   30   32   33   34   35   36   37   38   39   40   41
chain bonds :
    8-9   9-45   11-13   11-12   11-47   12-29   13-14   14-30   14-31   15-16   16-17
    17-18   17-19   18-24   18-25   25-26   31-42   45-46   46-47
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   29-32   29-36   30-37   30-41   32-33   33-34
    34-35   35-36   37-38   38-39   39-40   40-41
exact/norm bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   8-9   9-45   11-13   11-12   11-47   12-29   13-14
    14-30   14-31   15-16   16-17   17-18   17-19   18-24   18-25   25-26   31-42   45-46
    46-47
normalized bonds :
    29-32   29-36   30-37   30-41   32-33   33-34   34-35   35-36   37-38   38-39   39-40
    40-41

G1:C,N

G2:C,O,S,N

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   8:CLASS   9:CLASS   11:CLASS
    12:CLASS   13:CLASS   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
    19:CLASS   24:CLASS   25:CLASS   26:CLASS   29:Atom   30:Atom   31:CLASS   32:Atom
    33:CLASS   34:CLASS   35:Atom   36:Atom   37:Atom   38:Atom   39:Atom   40:Atom
    41:Atom   42:CLASS   45:CLASS   46:CLASS   47:CLASS